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INVESTIGATION OF THE DENSITY OF STATE PROBABILITY FOR FE METAL CONTACT TO TIO2 SEMICONDUCTOR SYSTEM

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Abstract

In this paper, the density of state (DOS) at Fe metal contact to Titanium dioxide semiconductor (TiO_2) has been studied and investigated using quantum consideration approaches. The study and calculations of (DOS) depended on the orientation Λ_{ms} and driving Δ^0 energies. Λ_{ms} was a function of TiO_2 and Fe materials' refractive index and dielectric constant. Attention has focused on the effect of Λ_{ms} on the characteristic of (DOS), which increased with the increasing of refractive index and dielectric constant of Fe metal and vice versa. The results of (DOS) and its relation with Λ_{ms} and Δ^0 values of system have been discussed. As Λ_{ms} for contact system is increased, (DOS) values increased at first, but the relation is disturbed later and transforms into an inverse proportion as (DOS) values begin to decrease smoothly after reaching a certain point, e.g., at Δ^0 = 0.1 eV, the density reached its maximum point $1.10*10^{-1}$, then it steadily decreased.

Keywords: Density of State; Orientation Energy; Driving Energy; Fe Metal Contact to TiO2 System.

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Introduction

Electron transfer (ET) has been considered as a fundamental reaction underlying important processes in chemistry, physics, biophysics and applied science. This area of study includes atoms, molecules and large systems[1]. The electron transfer processes have involved an electron that can be transferred from a metal to a semiconductor surface in a variety of applied devices[2]. The density of states (DOS) for physical and condensed matter systems is the proportion of states to occupy by the system at each energy, it's represented as a distribution of probability. The density of states at the interface of metal-semiconductor structures is the main characteristic of electron transfer[3]. However, the density of states are covered the band energy at metal and included the conduction and valence bands at the metal-semiconductor. The cross-sectional geometry introduces much more information on the atomic structure at the metal-semiconductor interface, e.g., applying atomically resolved cross-sectional and exploring the density of states at the atomic scale[4]. As Marcus recognized the importance of the variations in nuclear structure between the reactants and the products as well as the solvent contribution to the ET rate [3], this model was broadened to describe transferring an electron from a single donor state into a continuum[5]. Since the pioneering work describing the dynamics of the ET reaction in the early 1980s, a lot of theoretical effort has been made to explain the mechanisms of the electron transfer[6]. The detailed analytical theory has progressed considerably in the field of electron transfer in the past half-century depending on Marcus's theory and the implementation of new technologies[7]. In previous years, several researchers have investigated the electron transfer kinetics at the interface between metal and semiconductor[8]. They proved that electron transfer in a surface plasmon band from the semiconductor to the metal is achieved within a time period of a laser pulse. Interfaces formation on the basis of Metal/Semiconductor contact in 2009[9], gave basic features of many metal /semiconductor devices. The importance of the investigation of the interface's states formation is included in the fact that the fewer densities of the interface states require to provide an appropriate ET in devices and to guarantee control of the potential[10]. An electron transfer simulation was achieved at an electronic nanodevices system. It's revealed that rate constant for metal - semiconductors, in general, depends on electronic concentration, coupling transition coefficient, work function, transition energy, affinity, volume of the unit cell and the temperature[11]. In addition to the electronic transport parameters, it has been found that the probability of electron transfer is relative to the coupling coefficient that results from the overlap between wave functions for Metal/Semiconductors interfaces and which limits the transition by tunneling between the two different materials[12]. As well known, the construction of the metal/semiconductor contact based on the alignment of the energy bands diagram has introduced intimate interaction between metal and semiconductor and the ET systems that are considered in general as a fundamental phenomenon for technology[13]. The analysis of the probability of ET and its cross-section at any physical systems depending on a perturbation theory, allows us to investigate and evaluate the amount of the rate constant of the electron transfer range in technological devices. In fact, the interface charge transfer includes several major applications, for example, quantum confinement devices, solar cells, etc[14].

Based on experimental data, we'll focus on the study of (DOS) for a new different contact system (Fe/TiO_2) to explore the nature of relations between contact parameters that control ET conditions and compare them with the results obtained from previous researches.

This paper is an attempt to build an extensive future study on the rest of the factors that cover ET processes, i.e., potential barrier high, the rate constant of ET, lifetime, and the cross-section.

1. Theoretical model

The (DOS) describes the number of states available in metal-semiconductor system. It's essential to determine the distribution of electron transition that's move from metal to semiconductor in a system. The quantum density operator is an operator that evidently written in general form[15]:

$$\hat{D}(E_i) = \sum_i |\varphi_i(t)\rangle \hat{d}_i \langle\varphi_i(t)| \quad \text{..... (1)}$$

Where $\hat{d}_i$ is the density operator will be evidently to $\sum_i \hat{d}_i^{\,2} \leq 1$ [16]and $|\varphi_i(t)\rangle$ is the wave functions for electrons satisfies the orthonormal conditions $\langle\varphi_i(t)\,|\varphi_j(t)\rangle = \delta_{ij}(t)$ [17].The complete set basis $|\varphi_m(t)\ \rangle$, and $|\varphi_s(t)\rangle$ for metal and semiconductor system can be formulated as:

$$|\varphi_m(t)\ \rangle = \sum_j^{\infty} C_{m_j} \left|\varphi_{m_j}\ \right\rangle \text{.....(2)}$$

And:

$$|\varphi_s(t)\rangle = \sum_j^{\infty} C_{s_j} \left|\varphi_{s_j}\right\rangle \text{.....(3)}$$

Where C_{m_i} and C_{s_i} are the amplitude of wave functions for metal and semiconductor respectively. So far, under the expectation values rule, it can be carried out due to set of wave functions $|\varphi_m(t)\rangle$, and $|\varphi_s(t)\rangle$ [18]:

$$\langle\hat{D}(E_i)\rangle = \sum_i^{\infty}\sum_j^{\infty} \langle\varphi_i(t)|\varphi_s(t)\ \rangle \langle\varphi_s(t)\ |\hat{D}(E_i)|\varphi_m(t)\ \rangle \langle\varphi_m(t)\ |\varphi_i(t)\rangle \text{...(4)}$$

Moreover, the overall density operator probability $\hat{D}(E_i)$ has been carried out to take a complicated form[19]:

$$\hat{D}(E_i) = e^{\frac{E}{k_B T}}\, D\ e^{\frac{-E}{k_B T}} \quad \text{..... (5)}$$

Where E is the energy of state, D represents the density of state value, k_B is the Boltzman constant and T is the temperature. So, by substituting Eq. (2) , Eq.(3) and Eq. (5) in Eq.(4) and simply to obtain:

$$\langle\hat{D}(E_i)\rangle = \sum_i^{\infty}\sum_j^{\infty} C_{s_j} \left\langle\varphi_i(t)\middle|\varphi_{s_j}\right\rangle C_{s_j}{}^{*} C_{m_j} e^{\frac{E_s}{k_B T}} \left\langle\varphi_{s_j}\middle|\ D\ \middle|\ \varphi_{m_j}\right\rangle e^{\frac{-E_m}{k_B T}} C_{m_j}{}^{*} \left\langle\ \varphi_{m_j}\middle|\varphi_i(t)\right\rangle$$
.....(6)

So under consideration $D_{ij} = C_{s_j}{}^{*} C_{m_j} \left\langle\varphi_{s_j}\middle|\ D\ \middle|\ \varphi_{m_j}\right\rangle$, the approximate solution:

$$\langle\hat{D}(E_i)\rangle = \sum_i^{\infty}\sum_j^{\infty} C_{s_j} \left\langle\varphi_i(t)\middle|\varphi_{s_j}\right\rangle e^{\frac{E_s}{k_B T}} D_{ij} e^{\frac{-E_m}{k_B T}} C_{m_j}{}^{*} \left\langle\ \varphi_{m_j}\middle|\varphi_i(t)\right\rangle \text{..... (7)}$$

The term of constants in the Eq.(7) above can be intensified and shorten into β_{ij} via:

$$\beta_{ij} = \left\langle\varphi_{s_j}\middle|C_{s_j}{}^{*}\varphi_i(t)\right\rangle^{*} C_{m_j}{}^{*} \left\langle\ \varphi_{m_j}\middle|\varphi_i(t)\right\rangle \text{..... (8)}$$

By inserting the β_{ij} over all states in the Eq. (7) to get:

$$\langle\hat{D}(E_i)\rangle = \sum_i^{\infty}\sum_j^{\infty} \beta_{ij} e^{\frac{-(E_m - E_s)}{k_B T}} \text{..... (9)}$$

The exact solution for Eq. (9) obtained would be proven by assuming that $\mathbb{A}_{ij} = \sum_i^{\infty} \sum_j^{\infty} \beta_{ij}$ and the effective energy $\Delta E_{ms} = (E_m - E_s)$ is a function of the energy levels for the two materials in system [17]. Then Eq. (9) reduced to constitute the basis:

$$\langle \hat{D}(E_i) \rangle = \mathbb{A}_{ij} e^{\frac{-\Delta E_{ms}}{k_B T}} \quad \text{..... (10)}$$

This activation energy of system ΔE_{ms} is connected to the reorientation energy of electron transfer Λ_{ms} and the standard driving energy Δ^0 of the electron transfer reaction processes due to the relation[20]:

$$\Delta E_{ms} = \frac{(\Lambda_{ms} + \Delta^0)^2}{4\Lambda_{ms}} \quad \text{..... (11)}$$

Inserting Eq.(11) in Eq.(10), and using trace technique for density of state operator $\hat{D}(E_i)$ to get the following expression:

$$\text{Trace}\langle \hat{D}(E_i) \rangle = \int_{+\infty}^{+\infty} \mathbb{A}_{ij} e^{-\frac{(\Lambda_{ms} + \Delta^0)^2}{4\Lambda_{ms} k_B T}} d\Delta^0 = 1 \quad \text{.....(12)}$$

By assuming that $c_1 = \frac{1}{4\Lambda_{ms} k_B T}$, and $c_2 = c_1(\Lambda_{ms} + \Delta^0)^2$, the integral in Eq.(12) will be solved using gamma function integral and produced that normalized constant will be:

$$\mathbb{A}_{ij} = \sqrt{\frac{1}{4\pi \Lambda_{ms} k_B T}} \quad \text{..... (13)}$$

Substituting the amplitude of density of state in Eq. (13) into the density of state expression in Eq.(10) produces:

$$\langle \hat{D}(E_i) \rangle = \sqrt{\frac{1}{4\pi \Lambda_{ms} k_B T}} e^{-\frac{(\Lambda_{ms} + \Delta^0)^2}{4\Lambda_{ms} k_B T}} \quad \text{..... (14)}$$

The orientation energy $\Lambda_{ms}(eV)$ is the energy needed to start electronic transfer in system, it is given by[21]:

$$\Lambda_{ms}(eV) = \frac{e^2}{4\pi\varepsilon_0}\left[\frac{1}{2r_s}\left(\frac{1}{n_s^2} - \frac{1}{\epsilon_s}\right) + \frac{1}{2r_m}\left(\frac{1}{n_m^2} - \frac{1}{\epsilon_m}\right) - \frac{\Lambda_{m-s}}{4R_s} - \frac{\Lambda_{s-m}}{4R_m} - \frac{2\Lambda_{m/s}}{\text{Rm}-s}\right] \text{..(15)}$$

where e is the electric charge, ε_0 is the permittivity, r_s and r_m are radii for semiconductor and metal respectively , n_s , n_m , ϵ_s and ϵ_s are the refractive index and dielectric constant for semiconductor and metal., R_s and R_m are the distance between semiconductor, metal and interface alternatively , R_{m-s} is the distance between semiconductor and metal.

The refractive index n_m of metal may be calculated using absolute value, it's given in the form[22]:

$$|n_m| = n_m . {n_m}^* = \sqrt{N^2 + k^2} \quad \text{.....(16)}$$

Where $n_m = N + ik$ and ${n_m}^* = N - ik$, N is the refraction coefficient and k is the extinction coefficient.

However, the dielectric constant of metal ϵ_m can by calculated using absolute value and given by[22]:

$$|\epsilon| = \epsilon\epsilon^* = \sqrt{{\epsilon_1}^2 + {\epsilon_2}^2} \quad \text{.....(17)}$$

Where $\epsilon_1 = N^2 - k^2$ and $\epsilon_2 = 2NK$ are dielectric parameters of metal

Moreover, the polarity function Λ_{m-s} of metal-semiconductor is:

$$\Lambda_{m-s} = \left(\frac{n_m^2 - n_s^2}{n_m^2 + n_s^2}\ \frac{1}{n_s^2} - \frac{\epsilon_m - \epsilon_s}{\epsilon_m + \epsilon_s}\ \frac{1}{\epsilon_s}\right) \text{.....(18)}$$

So, the polarity function Λ_{s-m} of semiconductor-metal can be presented as:

$$\Lambda_{s-m} = \left(\frac{n_s^2 - n_m^2}{n_s^2 + n_m^2}\ \frac{1}{n_m^2} - \frac{\epsilon_s - \epsilon_m}{\epsilon_s + \epsilon_m}\ \frac{1}{\epsilon_m}\right) \text{.....(19)}$$

Furthermore, the polarity function $\Lambda_{m/s}$ for metal –semiconductor interface is equal to:

$$\Lambda_{m/s} = \left(\frac{1}{n_s^2 + n_m^2} - \frac{1}{\epsilon_s + \epsilon_m}\right) \text{.....(20)}$$

The radii of the metal or semiconductor should be estimated due to spherical approach[23]:

$$r_i = \left(\frac{3MW}{4\pi N_A \rho_{mas}}\right)^{\frac{1}{3}} \text{.....(21)}$$

Where MW is the molecular weight, ρ_{mas} is the mass density and N_A is Avogadro's number.

2. Results and Discussion

Due to the quantum consideration of electron transfer theory, (DOS) is investigated and calculated depending on Λ_{ms} for multi-identical electrons states in Fe metal contact to TiO_2 semiconductor system. The interface of the two materials is influenced strongly by Λ_{ms} and Δ^0 energies. This indicate that ET is a function of the radii and polarity index of both materials. Using MATLAB version R2014a, (DOS) of the Fe contact to TiO_2 semiconductor was theoretically calculated as a function of the Λ_{ms} in Eq.(14), which describes the distribution of electrons in the system. Furthermore, we evaluated the radii of Fe and TiO_2 by inserting in Eq.(21) the mass density $\rho = 7.874\ g/cm^3$, molecular weight M=55.845 g/mol for Fe metal and the $\rho = 4.230\ g/cm^3$, molecular weight M=79.866 g/mol for TiO_2 materials from Tab.1 with Avogadro's constant of $N_A = 6.02 \times 10^{23}\ \frac{Molecule}{mol}$. The results are $r_{Fe} = 1.411\ A^0$ and $r_{TiO2} = 1.95\ A^0$ for Fe and TiO_2 respectively.

Table 1: Properties of TiO2 semiconductor[24, 25].

Properties	TiO2
Molecular weight g/mol	79.866
Dielectric Constant	55
Mass Density (g/cm^3)	4.23
Density of state Ns /cm^3)	1.163×10^{25}
Crystal structure	Tetragonal rutile
Refractive index	2.609
Lattice constant(Å)	a = 4.5936 ,c =2.9587
Radius(Å)	1.9563
Conduction band energy(eV)	4.05
Energy gab (eV)	3.2 eV
Refractive index	2.5688
Electron concentration (1/cm^3)	2×10^{20}
Electron affinity (eV)	4.2

The refractive index of Fe metal is calculated using Eq.(16) with refraction coefficient N and extinction coefficient k that listed with the results in Tab.2.

Table 2: The calculated refractive index for Fe metal.

Energy (ev)	Refraction index (N)	Extinction Coef. (K)	$n_m = N + iK$	$n_m^* = N - iK$	$\lvert n_m\rvert = \sqrt{N^2 + K^2}$
0.1	6.41	33.07	6.41+ 33.07i	6.41- 33.07i	33.68550133
0.15	6.26	22.82	6.26+ 22.82i	6.26-22.82i	23.66305137
0.2	3.68	18.23	3.68+ 18.23i	3.68-18.23i	18.59772298
0.26	4.98	13.68	4.98+ 13.68i	4.98-13.68i	14.55825539
0.3	4.87	12.05	4.87+ 12.05i	4.87-12.05i	12.99689963
0.36	4.68	10.44	4.68+ 10.44i	4.68-10.44i	11.44097898
0.4	4.42	9.75	4.42+ 9.75i	4.42-9.75i	10.70508758
0.5	4.14	8.02	4.14+ 8.02i	4.14-8.02i	9.025519376
0.6	3.93	6.95	3.93+ 6.95i	3.93-6.95i	7.984196891
0.7	3.78	6.17	3.78+ 6.17i	3.78-6.17i	7.235834437
0.8	3.65	5.6	3.65+ 5.6i	3.65-5.6i	6.684496989
0.9	3.52	5.16	3.52+5.16i	3.52-5.16i	6.246278892
1	3.43	4.79	3.43+4.79i	3.43-4.79i	5.89143446
1.1	3.33	4.52	3.33+4.52i	3.33-4.52i	5.614205198
1.2	3.24	4.26	3.24+4.26i	3.24-4.26i	5.352121075
1.3	3.16	4.07	3.16+4.07i	3.16-4.07i	5.15271773
1.4	3.12	3.87	3.12+3.87i	3.12-3.87i	4.971046168
1.5	3.05	3.77	3.05+3.77i	3.05-3.77i	4.849267986
1.6	3	3.6	3+3.6i	3-3.6i	4.686149806
1.7	2.98	3.52	2.98+3.52i	2.98-3.52i	4.612027754
1.8	2.92	3.46	2.92+3.46i	2.92-3.46i	4.527471701
1.9	2.89	3.37	2.89+ 3.37i	2.89-3.37i	4.439481952
2	2.85	3.36	2.85+3.36i	2.85-3.36i	4.405916477
2.1	2.8	3.34	2.8+ 3.34i	2.8-3.34i	4.3583942
2.2	2.74	3.33	2.74+3.33i	2.74-3.33i	4.31236594

2.3	2.65	3.34	2.65+3.34i	2.65-3.34i	4.263578309
2.4	2.56	3.31	2.56+3.31i	2.56-3.31i	4.184459344
2.5	2.46	3.31	2.46+3.31i	2.46-3.31i	4.124039282
2.6	2.34	3.3	2.34+3.3i	2.34-3.3i	4.045441879
2.7	2.23	3.25	2.23+3.25i	2.23-3.25i	3.941497177
2.8	2.12	3.23	2.12+3.23i	2.12-3.23i	3.863586417
2.9	2.01	3.17	2.01+3.17i	2.01-3.17i	3.75353167
3	1.88	3.12	1.88+3.12i	1.88-3.12i	3.642636408
3.1	1.78	3.04	1.78+3.04i	1.78-3.04i	3.522782991
3.2	1.7	2.96	1.7+2.96i	1.7-2.96i	3.413444009
3.3	1.62	2.87	1.62+2.87i	1.62-2.87i	3.295648646
3.4	1.55	2.79	1.55+2.79i	1.55-2.79i	3.191645344
3.5	1.5	2.7	1.5+2.7i	1.5-2.7i	3.088689042
3.6	1.47	2.63	1.47+2.63i	1.47-2.63i	3.012938765
3.7	1.43	2.56	1.43+2.56i	1.43+2.56i	2.932319901
3.83	1.38	2.49	1.38+2.49i	1.38-2.49i	2.846840354
4	1.3	2.39	1.3+2.39i	1.3-2.39i	2.720680062
4.17	1.26	2.27	1.26+2.27i	1.26-2.27i	2.596247292
4.33	1.23	2.18	1.23+2.18i	1.23-2.18i	2.50305813
4.5	1.2	2.1	1.2+2.1i	1.2-2.1i	2.418677324
4.67	1.16	2.02	1.16+2.02i	1.16-2.02i	2.329377599
4.83	1.14	1.93	1.14+1.93i	1.14-1.93i	2.241539649
5	1.14	1.87	1.14+1.87i	1.14+1.87i	2.190091322
5.17	1.12	1.81	1.12+1.81i	1.12-1.81i	2.128497122
5.33	1.11	1.75	1.11+1.75i	1.11-1.75i	2.072341671
5.5	1.09	1.17	1.09+1.17i	1.09-1.17i	1.599062225
5.67	1.09	1.65	1.09+1.65i	1.09-1.65i	1.977523704
5.83	1.1	1.61	1.1+1.61i	1.1-1.61i	1.949897433
6	1.09	1.59	1.09+1.59i	1.09-1.59i	1.927744796
6.17	1.08	1.57	1.08+1.57i	1.08-1.57i	1.905597019
6.33	1.04	1.55	1.04+1.55i	1.04-1.55i	1.866574402
6.5	1.02	1.51	1.02+1.51i	1.02-1.51i	1.822223916
6.67	1	1.47	1+1.47i	1-1.47i	1.77789201
6.83	0.97	1.43	0.97+1.43i	0.97-1.43i	1.727946758

The dielectric constant computed for different values of energy using Eq.(17) and the results listed in Tab.3.

Table 3: The calculated Dielectric constant and parameters for Fe metal.

Energy (ev)	Refraction index (N)	Extinction Coef. (K)	$\varepsilon_1 = N^2 - K^2$	$\varepsilon_2 = 2NK$	$\lvert\varepsilon\rvert = \varepsilon\varepsilon^* = \sqrt{\varepsilon_1^2 + \varepsilon_2^2}$
0.1	6.41	33.07	-1052.5368	423.9574	1134.713
0.15	6.26	22.82	-481.5648	285.7064	559.94
0.2	3.68	18.23	-318.7905	134.1728	345.8753
0.26	4.98	13.68	-162.342	136.2528	211.9428
0.3	4.87	12.05	-121.4856	117.367	168.9194
0.36	4.68	10.44	-87.0912	97.7184	130.896
0.4	4.42	9.75	-75.5261	86.19	114.5989
0.5	4.14	8.02	-47.1808	66.4056	81.46
0.6	3.93	6.95	-32.8576	54.627	63.7474
0.7	3.78	6.17	-23.7805	46.6452	52.3573
0.8	3.65	5.6	-18.0375	40.88	44.6825
0.9	3.52	5.16	-14.2352	36.3264	39.016
1	3.43	4.79	-11.1792	32.8594	34.709
1.1	3.33	4.52	-9.3415	30.1032	31.5193
1.2	3.24	4.26	-7.65	27.6048	28.6452
1.3	3.16	4.07	-6.5793	25.7224	26.5505
1.4	3.12	3.87	-5.2425	24.1488	24.7113
1.5	3.05	3.77	-4.9104	22.997	23.5154
1.6	3	3.6	-3.96	21.6	21.96
1.7	2.98	3.52	-3.51	20.9792	21.2708
1.8	2.92	3.46	-3.4452	20.2064	20.498
1.9	2.89	3.37	-3.0048	19.4786	19.709
2	2.85	3.36	-3.1671	19.152	19.4121
2.1	2.8	3.34	-3.3156	18.704	18.9956
2.2	2.74	3.33	-3.5813	18.2484	18.5965
2.3	2.65	3.34	-4.1331	17.702	18.1781
2.4	2.56	3.31	-4.4025	16.9472	17.5097
2.5	2.46	3.31	-4.9045	16.2852	17.0077
2.6	2.34	3.3	-5.4144	15.444	16.3656
2.7	2.23	3.25	-5.5896	14.495	15.5354
2.8	2.12	3.23	-5.9385	13.6952	14.9273
2.9	2.01	3.17	-6.0088	12.7434	14.089
3	1.88	3.12	-6.2	11.7312	13.2688
3.1	1.78	3.04	-6.0732	10.8224	12.41
3.2	1.7	2.96	-5.8716	10.064	11.6516
3.3	1.62	2.87	-5.6125	9.2988	10.8613
3.4	1.55	2.79	-5.3816	8.649	10.1866
3.5	1.5	2.7	-5.04	8.1	9.54
3.6	1.47	2.63	-4.756	7.7322	9.0778
3.7	1.43	2.56	-4.5087	7.3216	8.5985
3.83	1.38	2.49	-4.2957	6.8724	8.1045
4	1.3	2.39	-4.0221	6.214	7.4021
4.17	1.26	2.27	-3.5653	5.7204	6.7405
4.33	1.23	2.18	-3.2395	5.3628	6.2653
4.5	1.2	2.1	-2.97	5.04	5.85

4.67	1.16	2.02	-2.7348	4.6864	5.426
4.83	1.14	1.93	-2.4253	4.4004	5.0245
5	1.14	1.87	-2.1973	4.2636	4.7965
5.17	1.12	1.81	-2.0217	4.0544	4.5305
5.33	1.11	1.75	-1.8304	3.885	4.2946
5.5	1.09	1.17	-0.1808	2.5506	2.557
5.67	1.09	1.65	-1.5344	3.597	3.9106
5.83	1.1	1.61	-1.3821	3.542	3.8021
6	1.09	1.59	-1.34	3.4662	3.7162
6.17	1.08	1.57	-1.2985	3.3912	3.6313
6.33	1.04	1.55	-1.3209	3.224	3.4841
6.5	1.02	1.51	-1.2397	3.0804	3.3205
6.67	1	1.47	-1.1609	2.94	3.1609
6.83	0.97	1.43	-1.104	2.7742	2.9858

Depending on the refractive indices n_m and static dielectric constants ε_m for the Fe metal from Tabs 2 and 3 and for TiO_2 Tab.1 and taken the results of radii for both materials and the distances $R_s = 2.956\ A^0$, $R_m = 2.411\ A^0$ for semiconductor and metal and interface $R_{m-s} = 3.368\ A^0$ and taken $\frac{\Delta e^2}{4\pi\epsilon_0} = 14.4(eV)$, then using all these data in Eq.(15) to evaluate Λ_{ms} for Fe metal contact with TiO_2 semiconductor in Fe/ TiO_2 systems. The obtained results are listed in Tab.4.

Table 4: The orientation energy for Fe/ TiO2 contact system.

$\lvert n_m \rvert$	$\lvert \varepsilon \rvert$	$\Lambda_{ms}(eV)$
33.68550133	1134.713	0.32828899
23.66305137	559.94	0.327965715
18.59772298	345.8753	0.327328396
14.55825539	211.9428	0.325803716
12.99689963	168.9194	0.324545914
11.44097898	130.896	0.322473462
10.70508758	114.5989	0.321030329
9.025519376	81.46	0.315793306
7.984196891	63.7474	0.310264875
7.235834437	52.3573	0.304465282
6.684496989	44.6825	0.298764468
6.246278892	39.016	0.293074808
5.89143446	34.709	0.287518672
5.614205198	31.5193	0.282464383
5.352121075	28.6452	0.277011232
5.15271773	26.5505	0.272360549
4.971046168	24.7113	0.267699691
4.849267986	23.5154	0.264327847
4.686149806	21.96	0.259472773
4.612027754	21.2708	0.257129973
4.527471701	20.498	0.254346999

4.439481952	19.709	0.251320511
4.405916477	19.4121	0.250129628
4.3583942	18.9956	0.24840818
4.31236594	18.5965	0.246700422
4.263578309	18.1781	0.24484576
4.184459344	17.5097	0.241737656
4.124039282	17.0077	0.239277719
4.045441879	16.3656	0.235961489
3.941497177	15.5354	0.2313655
3.863586417	14.9273	0.227756634
3.75353167	14.089	0.222407722
3.642636408	13.2688	0.216705975
3.522782991	12.41	0.210172427
3.413444009	11.6516	0.203858238
3.295648646	10.8613	0.196658949
3.191645344	10.1866	0.189945116
3.088689042	9.54	0.18295518
3.012938765	9.0778	0.177586888
2.932319901	8.5985	0.171658001
2.846840354	8.1045	0.165123505
2.720680062	7.4021	0.155002096
2.596247292	6.7405	0.144451604
2.50305813	6.2653	0.136177
2.418677324	5.85	0.128408575
2.329377599	5.426	0.119903931
2.241539649	5.0245	0.111259062
2.190091322	4.7965	0.106069904
2.128497122	4.5305	0.099738791
2.072341671	4.2946	0.0938576
1.599062225	2.557	0.040920946
1.977523704	3.9106	0.083702952
1.949897433	3.8021	0.080694082
1.927744796	3.7162	0.078265845
1.905597019	3.6313	0.075824744
1.866574402	3.4841	0.071492377
1.822223916	3.3205	0.066522574
1.77789201	3.1609	0.06150969
1.727946758	2.9858	0.055813202

Furthermore, (DOS) or $\langle \widehat{D}(E_i) \rangle$ of the Fe/TiO2 systems is calculated according to Eq.(14) by using MATLAB program and taking different values of free energy Δ^0= 0.05, 0.1, 0.15 and 0.2eV and inserting the values of Λ_{ms} from Tab.4. The results are included in Tab.5 and illustrated in figure (1).

Table 5: The DOS data for Fe/ TiO2 contact system.

The density of state $\langle \widehat{D}(E_i) \rangle$			
The driving free energy Δ^0 (eV)			
0.05	0.1	0.15	0.2
3.98E-02	1.17E-02	2.93E-03	6.33E-04
4.00E-02	1.17E-02	2.94E-03	6.34E-04
4.03E-02	1.18E-02	2.96E-03	6.38E-04
4.10E-02	1.20E-02	3.00E-03	6.45E-04
4.16E-02	1.21E-02	3.04E-03	6.52E-04
4.25E-02	1.24E-02	3.10E-03	6.62E-04
4.32E-02	1.26E-02	3.14E-03	6.69E-04
4.59E-02	1.33E-02	3.30E-03	6.97E-04
4.89E-02	1.41E-02	3.47E-03	7.26E-04
5.22E-02	1.50E-02	3.66E-03	7.58E-04
5.57E-02	1.59E-02	3.86E-03	7.90E-04
5.94E-02	1.69E-02	4.06E-03	8.23E-04
6.33E-02	1.79E-02	4.27E-03	8.55E-04
6.71E-02	1.89E-02	4.47E-03	8.85E-04
7.14E-02	2.00E-02	4.69E-03	9.18E-04
7.53E-02	2.10E-02	4.89E-03	9.46E-04
7.95E-02	2.21E-02	5.10E-03	9.75E-04
8.26E-02	2.29E-02	5.25E-03	9.96E-04
8.74E-02	2.41E-02	5.47E-03	1.03E-03
8.98E-02	2.47E-02	5.58E-03	1.04E-03
9.27E-02	2.54E-02	5.72E-03	1.06E-03
9.60E-02	2.62E-02	5.86E-03	1.08E-03
9.74E-02	2.65E-02	5.92E-03	1.08E-03
9.93E-02	2.70E-02	6.01E-03	1.09E-03
1.01E-01	2.75E-02	6.10E-03	1.10E-03
1.04E-01	2.80E-02	6.19E-03	1.11E-03
1.07E-01	2.90E-02	6.35E-03	1.13E-03
1.10E-01	2.97E-02	6.48E-03	1.15E-03
1.15E-01	3.07E-02	6.66E-03	1.17E-03
1.21E-01	3.22E-02	6.91E-03	1.19E-03
1.26E-01	3.34E-02	7.11E-03	1.21E-03
1.35E-01	3.53E-02	7.41E-03	1.24E-03
1.44E-01	3.75E-02	7.74E-03	1.27E-03
1.55E-01	4.00E-02	8.12E-03	1.30E-03
1.67E-01	4.26E-02	8.50E-03	1.32E-03
1.82E-01	4.58E-02	8.93E-03	1.35E-03
1.98E-01	4.90E-02	9.33E-03	1.37E-03
2.15E-01	5.25E-02	9.75E-03	1.38E-03
2.29E-01	5.53E-02	1.01E-02	1.38E-03
2.46E-01	5.85E-02	1.04E-02	1.38E-03
2.66E-01	6.22E-02	1.07E-02	1.37E-03

3.01E-01	6.83E-02	1.12E-02	1.33E-03
3.43E-01	7.50E-02	1.16E-02	1.27E-03
3.79E-01	8.05E-02	1.18E-02	1.20E-03
4.18E-01	8.57E-02	1.19E-02	1.12E-03
4.64E-01	9.13E-02	1.18E-02	1.01E-03
5.17E-01	9.69E-02	1.16E-02	8.84E-04
5.51E-01	1.00E-01	1.13E-02	8.00E-04
5.97E-01	1.03E-01	1.09E-02	6.92E-04
6.42E-01	1.06E-01	1.03E-02	5.88E-04
1.17E+00	6.89E-02	1.19E-03	6.10E-06
7.29E-01	1.09E-01	9.04E-03	4.11E-04
7.57E-01	1.10E-01	8.59E-03	3.61E-04
7.80E-01	1.10E-01	8.19E-03	3.22E-04
8.03E-01	1.10E-01	7.78E-03	2.85E-04
8.47E-01	1.09E-01	6.99E-03	2.22E-04
8.99E-01	1.07E-01	6.02E-03	1.59E-04
9.53E-01	1.04E-01	4.99E-03	1.07E-04
1.02E+00	9.75E-02	3.82E-03	6.11E-05
1.07E+00	9.10E-02	2.94E-03	3.58E-05
1.12E+00	8.14E-02	2.01E-03	1.68E-05
1.16E+00	7.04E-02	1.28E-03	6.94E-06
1.19E+00	6.03E-02	8.11E-04	2.90E-06
1.21E+00	5.22E-02	5.38E-04	1.33E-06
1.22E+00	4.65E-02	3.93E-04	7.34E-07
1.22E+00	3.80E-02	2.28E-04	2.63E-07

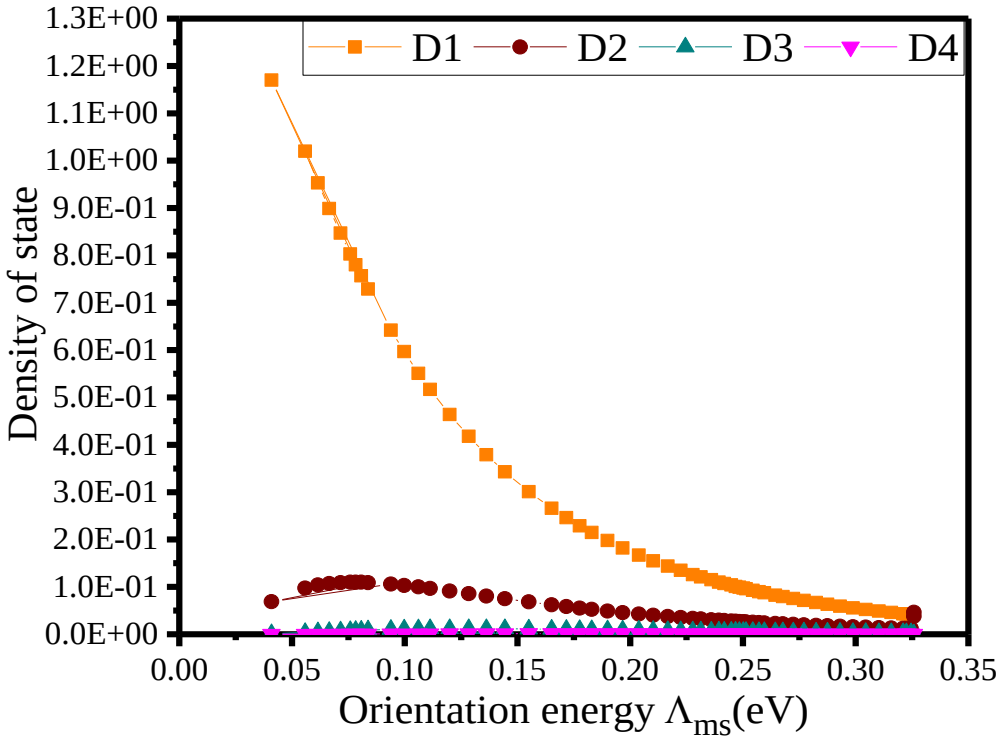

Figure-1: The relation between Λ_{ms} and (DOS) for $\Delta^0 = 0.05, 0.1, 0.15$ *and* 0.2 *eV* of Fe/TiO_2 contact system.

The characteristic of (DOS) have been calculated and investigated theoretically according to the quantum transition theory. It's a common to consider that Λ_{ms} and Δ^0 are the main parameters to the electronic (DOS) expression in Eq.(14). The electronic (DOS) was performed to provide insight into the electrical properties of Fe contact to TiO_2.

The Λ_{ms} has evaluated via optical refractive index and dielectric constant of the system. As seen in Eq.(16) and Eq.(17), the refractive index and dielectric constant are mainly related to refraction coefficient N and the extinction coefficient K of Fe metal. It has been shown in Tab.2 that n_m is inversely proportional to E, while it is directly proportional to the refraction coefficient N. On the other hand, n_m is increased with the increasing of the extinction coefficient k**.** However, the data in Tab.3 showed that ε_m values are increased with the increase of K. As observed, Λ_{ms} in Tab.4 is increased with the increasing both parameters; the dielectric constant and the refractive index of Fe metal. From Tab.5 and Fig.1, it is noticed that the electronic density values are increased firstly with the increasing of Λ_{ms}, and the relation is disturbed later and turns into an inverse proportion as (DOS) values begin to decrease smoothly after reaching a certain point, e.g., at Δ^0 =0.1 eV, the density reached its maximum point $1.10*10^{-1}$, then it steadily decreased. This is happened because the increasing of Λ_{ms} at the first, made the configuration of energy levels for the Fe - TiO_2 system more aligned to each other, i.e., the donor and acceptor are more closed before the electronic transfer process happens. After that, the increase in Λ_{ms} values causes a deformation in the contact system, and then decreasing the density of state probability. Furthermore, for this system, the increase in driving energy led to a decrease in the density of electronic state.

As it was found from the results of the current research, that the relation between DOS and Λ_{ms} is generally an inverse proportion relationship, and this is consistent with the results of previous researchs [11], [12] and [24].

3. Conclusions

In conclusion, the density of state in Fe contact to TiO_2 is forcedly relative to Λ_{ms} and Δ^0 energies. The (DOS) characteristics limits the electron transfer current and electronic cross-section based on Λ_{ms} and Δ^0 energies variations. Basically, due to quantum consideration, the relation between the $\langle \widehat{D}(E_i) \rangle$ and Λ_{ms} is characterized by an exponential form, that's showed in Tab.5 and figure (1), and it's because the strength coupling and the alignment of energy levels between Fe metal and TiO_2 semiconductor.

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